

Adaptive Error Covariances Estimation Methods for Ensemble Kalman Filters

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Abstract

This paper presents a computationally fast algorithm for estimating, both, the system and observation noise covariances of nonlinear dynamics, that can be used in an ensemble Kalman filtering framework. The new method is a modification of Belanger's recursive method, to avoid an expensive computational cost in inverting error covariance matrices of product of innovation processes of different lags when the number of observations becomes large. When we use only product of innovation processes up to one-lag, the computational cost is indeed comparable to a recently proposed method by Berry-Sauer's. However, our method is more flexible since it allows for using information from product of innovation processes of more than one-lag.

Extensive numerical comparisons between the proposed method and both the original Belanger's and Berry-Sauer's schemes are shown in various ex-

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amples, ranging from low-dimensional linear and nonlinear systems of SDE's and 40-dimensional stochastically forced Lorenz-96 model. Our numerical results suggest that the proposed scheme is as accurate as the original Belanger's scheme on low-dimensional problems and has a wider range of more accurate estimates compared to Berry-Sauer's method on L-96 example.

Keywords: ensemble Kalman filter, adaptive covariance estimation, QR estimation method

1. Introduction

Ensemble Kalman filters (EnKF) are ubiquitous in data assimilation of high-dimensional nonlinear problems [1, 2], particularly, it has received serious attentions in weather forecasting application [3]. While this practical method has been successful in applications, the accuracy of the resulting estimates is mostly determined by the prescription of both the system and observation error covariance statistics in the absence of model error. In fact, obtaining accurate covariance statistical estimates is still a challenging problem. Recent study [4] suggested that one should be cautious in interpreting the covariance estimates from approximate filtering methods, including EnKF.

Many numerical methods have been proposed to improve the filter covariance estimates. For example, a naive strategy is to directly inflate the covariance statistics with an empirically chosen inflation factor [5, 6, 7], while a second class of strategy is to use the current observations to adaptively inflate/tune the covariance statistics [8, 9, 10, 11, 12, 13, 14, 15]. The central contribution of this paper is on a new adaptive covariance estimation method

that can be used with EnKF. In particular, the new method is motivated by two recently developed EnKF-based covariance estimation methods [14, 15] that generalized, respectively, two competing methods that were introduced in early 70's for covariance estimation of stationary [8, 9] and time-varying linear problems [10]. All of these methods share a fundamental similarity, that is, they use the information from lag correlation of innovation processes (or prior forecast errors in the observation space) to approximate Q and R . While Berry-Sauer's estimation method [14] is computationally fast, their method used only product of innovation processes up to one-lag, $L = 1$, which by design, restricts its applicability especially when observations are sparse. Furthermore, the accuracy of the resulting estimates can be sensitive to the choice of a nuisance parameter, as we will show later. On the other hand, the covariance estimation method of [15], which is essentially Belanger's method implemented with EnKF [10], allows for using product of innovation processes of more than one-lag, $L > 1$, and produces estimates that converge faster. However, this method is computationally expensive when the number of observations, m , become large because it involves inversion of $m^2 \times m^2$ matrix for $L + 1$ times in each time step. This computational cost can be reduced from $\mathcal{O}((N_p m^6 + N_p^2 m^2 + N_p^3)L)$ to $\mathcal{O}((N_p m^3 + N_p^2 m^2 + N_p^3)L)$ by observing a special tensor structure of the covariance matrix, where N_p is the number of parameters for Q and R [11]. However, this reduced computational cost may still be unaffordable when the number of observations is large. In this paper, we present a new estimation method with computational cost $\mathcal{O}(m^2 N_p^2 (L + 1))$, that is faster than the Belanger's scheme when $N_p \ll m$, and more robust than Berry-Sauer's scheme [14] when observations

are sparse, and produces accurate estimates. We will provide the computational costs when these methods are used in tandem with ETKF ([2] version). We will refer to this new method as the modified Belanger’s method since it is motivated by the original Belanger’s formulation. We shall see that some aspect of the proposed method is also motivated by Berry-Sauer’s scheme.

The remainder of this paper is organized as follows: In Section 2, we will discuss the key idea behind the scheme and point out the similarities and differences between the proposed method with the existing schemes. This discussion is supported by two Appendices: Appendix A describes the detailed derivation and Appendix B provides pseudo-codes for an easy access to implementation. In particular, we will implement this scheme with ETKF that was used in [15], which was formulated by [2]. In Section 3 we show numerical results, comparing the proposed method with the original Belanger’s scheme implemented via ETKF [15] and Berry-Sauer’s scheme [14, 10] on various test models ranging from low-dimensional linear, low-dimensional nonlinear, and moderately higher-dimensional nonlinear stochastic filtering problems. We also include an experiment with LETKF [2] to demonstrate the potential for high-dimensional applications. We close the paper with a short summary and discussion in section 4.

2. Methodology

In this section, we present the mathematical formulation of a new method for estimating noise covariance matrices. Since the new method is motivated by earlier methods [10, 14, 16], we provide a short review of these existing methods and point out the similarities and differences. To simplify the pre-

sentation in this section, we assume that the observations are taken at every integration time step. We also provide the formulation for general case in which the observations are taken at every $N \geq 1$ integration time steps in Appendix A and the pseudo-algorithms in Appendix B.

2.1. Mathematical Formulation

We consider the following discrete-time linear filtering problem:

$$x_j = F_{j-1}x_{j-1} + \Gamma w_{j-1}, \quad (1)$$

$$y_j^o = H_j x_j + \xi_j, \quad (2)$$

where $x_j \in \mathbb{R}^n$ denotes the hidden state variable at time t_j . In (1), we assume that the dynamical model is driven by ℓ -dimensional independent identically distributed (i.i.d.) Gaussian noises w_{j-1} with known $\Gamma \in \mathbb{R}^{n \times \ell}$ and an unknown time-independent system error covariance matrix, $Q \in \mathbb{R}^{q \times q}$. The observations $y_j^o \in \mathbb{R}^m$ in (2) are corrupted by m -dimensional Gaussian i.i.d noises, ξ_j , with an unknown time-independent observation error covariance matrix, $R \in \mathbb{R}^{m \times m}$. Throughout this paper, we assume that F_j , H_j are linear operators independent of the system and observation noises. Our goal is to estimate the hidden state variable x_j and the noise covariance matrices, Q and R , given only noisy observations, y_j^o .

If the noise covariances Q and R are known, an unbiased optimal estimation (in the sense of minimum variance) for state x_j can be obtained by Kalman filter formula [17]. In particular, the Kalman filter formula recursively updates the prior mean and covariance estimates, x_j^f and B_j^f , respectively, of a conditional distribution $p(x_j | y_i^o, i \leq j-1)$, to the posterior mean and covariance estimates, x_j^a and B_j^a of a new conditional distribution

$p(x_j|y_i^o, i \leq j)$, incorporating the observation y_j^o at time t_j (see Appendix A for the detailed of the Kalman filter formula, cf. (28)).

Following the formulation in [10], we will use the *innovation process*, which is defined as the error of the prior mean estimates in the observation subspace,

$$v_j := y_j^o - H_j x_j^f = H_j \Delta x_j^f + \xi_j, \quad (3)$$

to estimate Q and R . In particular, Belanger's formulation relies on the description of prior forecast error with the following recursive equation [10],

$$\Delta x_j^f := x_j - x_j^f = \prod_{i=0}^{j-1} \mathcal{U}_i \Delta x_0^f - \mathcal{G}_{(j)}^\xi + \mathcal{F}_{(j)}^w, \quad (4)$$

where the explicit definition of the terms \mathcal{U}_j , $\mathcal{G}_{(j)}^\xi$, and $\mathcal{F}_{(j)}^w$, are presented in appendix A (cf. (33), (35), (36)). We remark that $\mathcal{G}_{(j)}^\xi$ and $\mathcal{F}_{(j)}^w$ are linear combinations of, respectively, ξ and w of previous time steps with coefficients involving F_{j-i} , H_{j-i} and the Kalman gain matrix K_{j-i} . Hence the coefficients of ξ in $\mathcal{G}_{(j)}^\xi$ and w in $\mathcal{F}_{(j)}^w$ are independent of the realization of ξ and w as long as the choice of Kalman gain matrix K_{j-i} at each time step is independent of ξ and w . However, this requirement can not be satisfied in any adaptive filter method which estimates Q and R sequentially since this estimation depends on the realization of ξ and w . In this situation, $\mathcal{G}_{(j)}^\xi$ and $\mathcal{F}_{(j)}^w$ are no longer linear functions of ξ and w . But they still can be viewed as linear combinations of ξ and w whose coefficients also involve ξ and w .

Taking the expectation of the product of (3) at different lags with respect

to realizations of ξ and w , we have:

$$\begin{aligned}
\mathbb{E}[v_j v_{j-l}^\top] &= H_j \mathbb{E}[\Delta x_j^f (\Delta x_{j-l}^f)^\top] H_{j-l}^\top + H_j \mathbb{E}[\Delta x_j^f \xi_{j-l}^\top] \\
&= H_j \left\{ \mathbb{E}[\mathcal{G}_{(j)}^\xi (\mathcal{G}_{(j-l)}^\xi)^\top] - \mathbb{E}[\mathcal{G}_{(j)}^\xi (\mathcal{F}_{(j-l)}^w)^\top] \right. \\
&\quad \left. - \mathbb{E}[\mathcal{F}_{(j)}^w (\mathcal{G}_{(j-l)}^\xi)^\top] + \mathbb{E}[\mathcal{F}_{(j)}^w (\mathcal{F}_{(j-l)}^w)^\top] \right\} H_{j-l}^\top \\
&\quad - H_j \mathbb{E}[\mathcal{G}_{(j)}^\xi \xi_{j-l}^\top] + H_j \mathbb{E}[\mathcal{F}_{(j)}^w \xi_j^\top] + \text{remainder terms}, \quad (5)
\end{aligned}$$

where all the terms that contain $\prod_{i=0}^{j-1} \mathcal{U}_i$ are absorbed in the remainder terms. When the filter is uniformly asymptotically stable, these remainder terms decay to zero at an exponential rate [10, 16]. If the Kalman gain matrices K_{j-i} are computed independently of ξ and w , the cross terms in (5) can be eliminated and the right hand side of (5) is a linear function of Q and R . Let's parameterize Q and R with N_Q and N_R parameters using some prescribed basis Q_s and R_s , respectively, such that:

$$Q = \sum_{s=1}^{N_Q} \alpha_s Q_s, \quad R = \sum_{s=1}^{N_R} \beta_s R_s.$$

Then, we can approximate (5) as follows,

$$\mathbb{E}[v_j v_{j-l}^\top] \approx \sum_{s=1}^{N_Q} \alpha_s \mathcal{H}_{j,l,s}^{(Q)} + \sum_{s=1}^{N_R} \beta_s \mathcal{H}_{j,l,s}^{(R)}, \quad (6)$$

where the explicit definition of $\mathcal{H}_{j,l,s}^{(Q)}$ and $\mathcal{H}_{j,l,s}^{(R)}$ are provided in Appendix A (cf. (43), (44)) and the approximation here is due to neglecting the remainder terms in (5).

In general situation when the Kalman gain matrix depends on the realization of ξ and w , the approximation in (6) is more than just due to neglecting the remainder terms. This is because the cross terms in (5) are not zero

and the right hand terms in (5) are no longer linear functions about Q and R . Now, let $\mathcal{E}_{j,l}$ be defined as the error of the approximation in (6). Taking average of these errors over time,

$$\begin{aligned} \frac{1}{J-L} \sum_{j=L+1}^J \mathcal{E}_{j,l} &:= \frac{1}{J-L} \sum_{j=L+1}^J \left(\mathbb{E}[v_j v_{j-l}^\top] - \left(\sum_{s=1}^{N_Q} \alpha_s \mathcal{H}_{j,l,s}^{(Q)} + \sum_{s=1}^{N_R} \beta_s \mathcal{H}_{j,l,s}^{(R)} \right) \right) \\ &= \frac{1}{J-L} \sum_{j=L+1}^J v_j v_{j-l}^\top - \frac{1}{J-L} \sum_{j=L+1}^J \delta_{j,l} \\ &\quad - \frac{1}{J-L} \sum_{j=L+1}^J \left(\sum_{s=1}^{N_Q} \alpha_s \mathcal{H}_{j,l,s}^{(Q)} + \sum_{s=1}^{N_R} \beta_s \mathcal{H}_{j,l,s}^{(R)} \right) \end{aligned} \quad (7)$$

where $\delta_{j,l} := v_j v_{j-l}^\top - \mathbb{E}[v_j v_{j-l}^\top]$. Suppose that the estimates for Q_j and R_j that are used to update the Kalman gain K_j equilibrate to some constant values. Then v_j is a stationary, Gaussian process with an exponential decay-ing correlation function $\|\mathbb{E}(v_i v_j^\top)\|_{\max} = \mathcal{O}(\exp(-\alpha|i-j|))$, where the order of magnitude is with respect to $|i-j|$. Then, it is not difficult to show that,

$$\mathbb{E} \left[\left(\frac{1}{J-L} \sum_{j=L+1}^J \delta_{j,l} \right) \left(\frac{1}{J-L} \sum_{i=L+1}^J \delta_{i,l} \right)^\top \right] = \mathcal{O} \left(\frac{1}{J-L} \right).$$

Secondly, the terms $\mathcal{E}_{j,l}$ are automatically eliminated when the Kalman gain matrices are updated with constant Q_j and R_j . Hence it is reasonable to believe that the variance and bias of $\frac{1}{J-L} \sum_{j=L+1}^J \mathcal{E}_{j,l}$ are small when Q_j and R_j vary slowly as functions of time, resulting to the following approximation,

$$\frac{1}{J-L} \sum_{j=L+1}^J v_j v_{j-l}^\top \approx \frac{1}{J-L} \sum_{j=L+1}^J \left(\sum_{s=1}^{N_Q} \alpha_s \mathcal{H}_{j,l,s}^{(Q)} + \sum_{s=1}^{N_R} \beta_s \mathcal{H}_{j,l,s}^{(R)} \right). \quad (8)$$

2.1.1. Modified Belanger's Method

Based on this observation, we propose the following method to estimate α_s and β_s :

- At the time point t_J , solve (8) for $\alpha_J := (\alpha_{1,J}, \dots, \alpha_{N_Q,J})$ and $\beta_J := (\beta_{1,J}, \dots, \beta_{N_R,J})$ using a least square method,

$$\min_{\alpha_J, \beta_J} \sum_{l=0}^L \left\| \sum_{j=L+1}^J v_j v_{j-l}^\top - \left\{ \sum_{s=1}^{N_Q} \alpha_{s,J} \left(\sum_{j=L+1}^J \mathcal{H}_{j,l,s}^{(Q)} \right) + \sum_{s=1}^{N_R} \beta_{s,J} \left(\sum_{j=L+1}^J \mathcal{H}_{j,l,s}^{(R)} \right) \right\} \right\| \quad (9)$$

where the new subscript J denotes the time t_J and the norm is Frobenius norm.

- Relax the estimates of α and β back to the estimates of the previous time step by the following running average:

$$\alpha_J = \alpha_{J-1} + \frac{1}{\tau}(\alpha_J - \alpha_{J-1}), \quad (10)$$

$$\beta_J = \beta_{J-1} + \frac{1}{\tau}(\beta_J - \beta_{J-1}), \quad (11)$$

where $\tau \geq 1$ is a nuisance parameter that will be empirically chosen.

We provide pseudo-algorithm 1 to guide the detail implementation of this method in Appendix B.

The idea of the first step of this method is to match the observed data $v_j v_{j-l}^\top$ with the estimation of its statistical mean in a least square manner since we have no access to $\mathbb{E}[v_j v_{j-l}^\top]$. A closely related method has been proposed by [16]. Specifically, their method can be thought of as the stationary version of this method. They assume stationarity of $v_j v_{j-l}^\top$ and use the ergodicity property to approximate $\mathbb{E}[v_j v_{j-l}^\top] \approx \frac{1}{J-L} \sum_{j=L+1}^J v_j v_{j-l}^\top$ in (6), and solve a different least square function,

$$\min_{\alpha_J, \beta_J} \sum_{l=0}^L \left\| \frac{1}{J-L} \sum_{j=L+1}^J v_j v_{j-l}^\top - \sum_{s=1}^{N_Q} \alpha_{s,J} \mathcal{H}_{l,s}^{(Q)} - \sum_{s=1}^{N_R} \beta_{s,J} \mathcal{H}_{l,s}^{(R)} \right\|, \quad (12)$$

where the norm is also taken to be the Frobenius norm. An important difference between this method and the modified Belanger's method in (9) is that the operators $\mathcal{H}^{(Q)}, \mathcal{H}^{(R)}$ in (12) are time independent and estimated separately assuming that the underlying processes are stationary [16]. However for any time-varying system their method is not applicable since we can't determine $\mathcal{H}^{(Q)}$ and $\mathcal{H}^{(R)}$. From this point of view, the modified Belanger's method is advantageous since it handles non-stationary cases by design.

The relaxation step (or the running average (10) and (11)), which was proposed in [14] for different reason, is included in this method to reduce the dependence of the Kalman gain matrices on ξ and w which subsequently reduce bias terms that can possibly occur when $\mathcal{E}_{j,l}$ and $\delta_{j,l}$ are large in (7). From the practical point of view, this relaxation step also increases the stability (or reduce the covariance) of the estimate.

2.1.2. The original Belanger's Method

The original Belanger's approach [10] mitigates the non-stationarity with a secondary Kalman filter, treating eqn (6) as an observation operator for Q and R . In particular, he assumes that the error in the approximation in (6) is white and normally distributed with mean zero and covariance $W_{j,l} \in \mathbb{R}^{m^2 \times m^2}$, obtained through a Gaussian approximation. Subsequently, a secondary Kalman filter is employed to solve the following optimization problem,

$$\min_{\alpha_J, \beta_J} \mathbf{Q}(\alpha_J, \beta_J) + \sum_{j=L+1, l=0}^{J, L} \left\| \text{vec}(v_j v_{j-l}^\top - \sum_{s=1}^{N_Q} \alpha_{s,J} \mathcal{H}_{j,l,s}^{(Q)} - \sum_{s=1}^{N_R} \beta_{s,J} \mathcal{H}_{j,l,s}^{(R)}) \right\|_{W_{j,l}^{-1}}^2, \quad (13)$$

where function \mathbf{Q} is any arbitrarily chosen positive definite quadratic function about $\alpha_J = (\alpha_{1,J}, \dots, \alpha_{N_Q,J})$ and $\beta_J = (\beta_{1,J}, \dots, \beta_{N_R,J})$ and the operator vec

denotes the vectorization of a matrix. Hence Belanger's method requires the inversion of $W_{j,l}$.

As mentioned in the introduction, this step of matrix inversion can be computed in $\mathcal{O}((N_p m^3 + N_p^2 m^2 + N_p^3)L)$ operations, realizing a special structure in W [11], where we define $N_p = N_Q + N_R$ as the total number of parameters. On the other hand, the cost of minimizing (9) in the modified Belanger's method requires only $\mathcal{O}(N_p^2 m^2 (L + 1))$. In the context of ETKF, both the modified and original Belanger's methods construct matrices (such as $\mathcal{H}^{(Q)}$ and $\mathcal{H}^{(R)}$) to be used in the secondary filter and the computational costs are $\mathcal{O}(nmN_e N_p (L + 1))$. Assuming that the observation error covariance R is diagonal, the cost of the primary filter (ETKF) is $\mathcal{O}(mN_e^2 + N_e^3 + nN_e^2)$ which is small compared to the total cost of the secondary filters; $\mathcal{O}((nmN_e N_p + N_p m^3 + N_p^2 m^2 + N_p^3)L)$ for the original Belanger's method and $\mathcal{O}((nmN_e N_p + N_p^2 m^2)(L + 1))$ for the modified Belanger's method. Setting the number of parameters to be less than the observations, $N_p \ll m$, then the second term $\mathcal{O}(N_p m^3 L)$ dominates the computational cost of the original Belanger's scheme if $m^2 \gg nN_e$. On the other hand, the second term in the computational estimate for the modified Belanger's scheme, $\mathcal{O}(N_p^2 m^2 L)$, is always less than the first term, $\mathcal{O}(nmN_e N_p L)$ whenever $N_p m \ll nN_e$.

Therefore, to achieve the most efficient computational cost with the modified Belanger's method, one should parameterize Q and R with a total number of parameters $N_p = N_Q + N_R$ that is less than the total number of observations, m , and choose an ensemble size, N_e , appropriately to satisfy $N_p m \ll nN_e$.

2.1.3. Berry-Sauer's Method

Finally, we will compare our method to a computationally faster, related, method that was recently proposed by [14]. This method is a variant of Mehra's method [8] for non-stationary (nonlinear) processes. In particular, their method is based on a formulation of the expectation of the product of innovations, $\mathbb{E}[v_j v_{j-l}^\top]$, that does not use the recursive identity in (4); resulting to a much simpler set of equations for zero-lag and one-lag products,

$$\mathbb{E}[v_j v_j^\top] = H_j B_j^f H_j^\top + R, \quad (14)$$

$$\mathbb{E}[v_{j+1} v_j^\top] + H_{j+1} F_j K_j \mathbb{E}[v_j v_j^\top] = H_{j+1} F_j (F_{j-1} B_{j-1}^a F_{j-1}^\top + \Gamma Q \Gamma^\top) H_j^\top,$$

where $B_j^f := \mathbb{E}[(x_j - x_j^f)(x_j - x_j^f)^\top]$ and $B_j^a := \mathbb{E}[(x_j - x_j^a)(x_j - x_j^a)^\top]$. The goal is to obtain Q and R , which are statistics of stationary processes w and ξ , respectively, from eqns (14) that involve statistics of non-stationary processes, namely, B_j^f, B_j^a, K_j . Furthermore, we have no access to the statistical quantities $\mathbb{E}[v_j v_j^\top]$ and $\mathbb{E}[v_{j+1} v_j^\top]$.

Their method consists of two steps: First, they estimate R and Q separately by solving,

$$R = v_j v_j^\top - H_j \tilde{B}_j^f H_j^\top, \quad (15)$$

and,

$$\min_{\alpha_j} \left\| v_{j+1} v_j^\top + H_{j+1} F_j K_j v_j v_j^\top - \sum_{s=1}^{N_Q} H_{j+1} F_j (F_{j-1} \tilde{B}_{j-1}^a F_{j-1}^\top + \alpha_{s,j} \Gamma Q_s \Gamma^\top) H_j^\top \right\|, \quad (16)$$

where they use parameterization $Q = \sum_{s=1}^{N_Q} \alpha_{s,j} Q_s$ with the Frobenius norm in the cost function above, and define $\alpha_j := (\alpha_{1,j}, \dots, \alpha_{N_Q,j})$. Additionally,

they use the covariance estimates from the Kalman filter formula as an approximation to the theoretical covariance estimates, $\tilde{B}_j^f \approx B_j^f$ and $\tilde{B}_j^a \approx B_j^a$. The second step in their method is to apply the moving average for the estimates of R and Q as in (10) to reduce the sensitivity (or variance) of the sequential estimates in (15) and (16) which depend on realization of noises w and ξ through $v_j v_j^\top$ and $v_{j+1} v_j^\top$. In some sense, this method is analogous to the original Belanger's method except that it uses moving average as the secondary filter rather than Kalman filter. This cheaper secondary filter is also adopted in the modified Belanger's scheme, replacing the expensive secondary Kalman filter. Thus, the computational cost of the modified Belanger's scheme is comparable to that of Berry-Sauer's method when the innovation lag, $L = 1$.

While this method is computationally the cheapest one relative to the other methods discussed in this paper, it is not clear that the approximations in (15) and (16) would induce bias in a long run. On the other hand, it is clear that bias indeed exists at any specific time point when the filter covariance estimates, $\tilde{B}_j^f \approx B_j^f$ and $\tilde{B}_j^a \approx B_j^a$, are sub-optimal since the endogenous variables in (15) and (16) depend on these covariances. On the other hand, the endogenous variables of both the modified and original Belanger's methods in (9) and (13), respectively, involve only $v_{j+l} v_j^\top$. We will numerically show in Section 3 that this method is more sensitive to the choice of the nuisance parameter τ in the relaxation step compared to the proposed modified Belanger's method and it requires large enough τ to reduce the variance of the error of the estimates which subsequently slows down the convergence of the estimates. One practical limitation of this method is

that it only uses information up to one-lag of innovation statistics which restricts its application when observations are sparse, as we will demonstrate in Section 3 below.

2.2. Covariance estimation with ensemble Kalman filters

The formulation of the covariance estimation method described in the previous section depends on knowing the linear operators F_j and H_j . For nonlinear problems, however, we typically know the nonlinear forward operator f_j and observational operator h_j instead of the linear operators. Here we will approximate the corresponding linear operators with an ensemble of solutions as in [14, 15] which is natural in the ensemble Kalman filtering setting.

More specifically, let $\{X_j^{a,i}\}_{i=1}^{N_e}$ be an ensemble of the posterior estimates of x_j and $X_{j+1}^{df,i} = f_j(X_j^{a,i})$ be the i -ensemble member of deterministic forecasts from initial condition $X_j^{a,i}$. Let U_j^a and U_{j+1}^{df} be matrices whose i th columns are the ensemble perturbations of $X_j^{a,i}$ and $X_{j+1}^{df,i}$ from their ensemble mean, respectively, then the linear forward operator F_j can be approximated by

$$F_j \approx U_j^{df} (U_j^a)^\dagger. \quad (17)$$

where \dagger denotes the matrix pseudo-inverse.

Similarly, let the prior ensemble be defined as $\{X_j^{f,i}\}_{i=1}^{N_e}$ of the stochastic system (these ensemble are Gaussian random samples with mean x_j^f and covariance P_j^f , cf. (19)). Also, let $Y_j^{f,i} = h_j(X_j^{f,i})$ be the i th ensemble member that is (nonlinearly) projected to the observational space. Define U_j^f and V_j^f as matrices whose i th columns consist of the ensemble perturbation of $X_j^{f,i}$

and $Y_j^{f,i}$ from its ensemble mean, respectively. Then the linear observation operator can be approximated by:

$$H_j \approx V_j^f (U_j^f)^\dagger. \quad (18)$$

Therefore, we can directly apply the new covariance estimation method discussed in Section 2.1.1 to update Q and R after each ensemble Kalman filter analysis step that updates the estimates of the state variables, x_j .

A second adjustment for using EnKF is in the generation of a new ensemble forecast that accounts for the stochastic terms once Q is updated. In particular, since

$$P_{j+1}^f = \frac{1}{N_e - 1} U_{j+1}^{df} (U_{j+1}^{df})^\top + \Gamma Q \Gamma^\top, \quad (19)$$

where Q is obtained from the covariance estimation method, then we need to construct matrix U_{j+1}^f such that $P_{j+1}^f = (N_e - 1)^{-1} U_{j+1}^f (U_{j+1}^f)^\top$. In the numerical experiments below, we use the method proposed in [15] which defines each column of U_{j+1}^f as an n -dimensional normally distributed random vector with mean zero and covariance P_{j+1}^f . In Algorithm 2 in the Appendix B, we will show the details of these adjustments for an implementation with Ensemble Transform Kalman Filter [18, 2].

For the implementation with LETKF in Section 3.4, we approximate F_j locally and we incorporate $\Gamma Q \Gamma^\top$ globally in the primary filter, even if the estimates of Q are obtained independently from the local secondary filter. In our implementation, we define the global estimate of Q to be the spatial average of local estimates of Q and we construct the global U_{j+1}^f by adding Gaussian random noises with mean zero and covariance $\Gamma Q \Gamma^\top$ to each column of the global prior ensemble perturbation, U_{j+1}^{df} . Also, in each local primary

filter analysis (LETKF) we use the global estimate of R (restricted to each local region), which we define as the spatial average of the local estimates of R that are obtained by independent local secondary filter.

3. Numerical Simulations

In this section, we will numerically compare the three methods discussed above, in particular, the proposed modified Belanger's scheme, the original Belanger's scheme, and Berry-Sauer's scheme on three simple models: 1) a two-dimensional linear model, 2) a low-dimensional nonlinear triad model, and 3) a stochastically forced 40-dimensional Lorenz-96 model. Finally, we will also compare results with LETKF, applying it to the Lorenz-96 model.

3.1. A linear example

In this section, we consider a two-dimensional linear filtering problem in (1) and (2) with parameters as in [10, 8],

$$F_j = \begin{pmatrix} 0.75 & -1.74 \\ 0.09 & 0.91 \end{pmatrix}, \Gamma = \begin{pmatrix} 1 & 0.4 \\ 0.1 & 1 \end{pmatrix}, Q = \mathcal{I}_2, R = 0.5\mathcal{I}_m.$$

In the simulations below, we will consider full and sparse observations. Full observations correspond to $H_j = \mathcal{I}_2$ and a 2×2 diagonal $R = 0.5\mathcal{I}_2$. On the other hand, sparse observations correspond to $H_j = [1, 0]$ and a scalar $R = 0.5$. Since Q and R are both diagonal matrices we naturally parameterize them by their diagonal components,

$$Q = \sum_{s=1}^{N_Q} \alpha_s Q_s, \quad R = \sum_{s=1}^{N_R} \beta_s R_s, \quad (20)$$

where in the case of full observations, $N_Q = N_R = 2$ and $Q_s = R_s \in \mathbb{R}^{2 \times 2}$ are matrices with one on the s th diagonal component and zero everywhere else. In the case of sparse observations $R_s = 1$ but Q_s remains the same. In the numerical simulations below, we will show results for 10000 and 50000 assimilation cycles for the cases of full and sparse observation, respectively.

In Figure 1 (left panel) we show the mean relative root-mean-square error of the estimates of diagonal components of Q and R as functions of time, from Berry-Sauer's method, the original Belanger's method, and the modified Belanger's method, respectively. The mean relative root-mean-square error is defined by

$$MRmse(t) = \frac{1}{n+m} \left(\sum_{s=1}^n \frac{|\tilde{Q}_{s,s,t} - Q_{s,s}|}{Q_{s,s}} + \sum_{s=1}^m \frac{|\tilde{R}_{s,s,t} - R_{s,s}|}{R_{s,s}} \right) \quad (21)$$

, where $\tilde{Q}_{s,s,t}$ are $\tilde{R}_{s,s,t}$ are the s th diagonal element of the estimates of Q and R at time t , respectively. In the estimation with Berry-Sauer's method, we use $\tau = 2000$ so that the variation of the estimation is small enough and we can see the estimates converge around the true value. On the other hand, we use $\tau = 1000$ in the estimation with the modified Belanger's method. For comparison purpose, we also use $L = 1$ for both the original and modified Belanger's method. Notice that while all three methods work reasonably well qualitatively, the errors of the modified and the original Belanger's methods are on the same order and smaller than that of the Berry-Sauer's method. In fact, the results are qualitatively similar when the number of lags are increased (results are not shown).

Now we check the sensitivity of both Berry-Sauer's method and the modified Belanger's method to the choice of the nuisance parameter, τ . In the

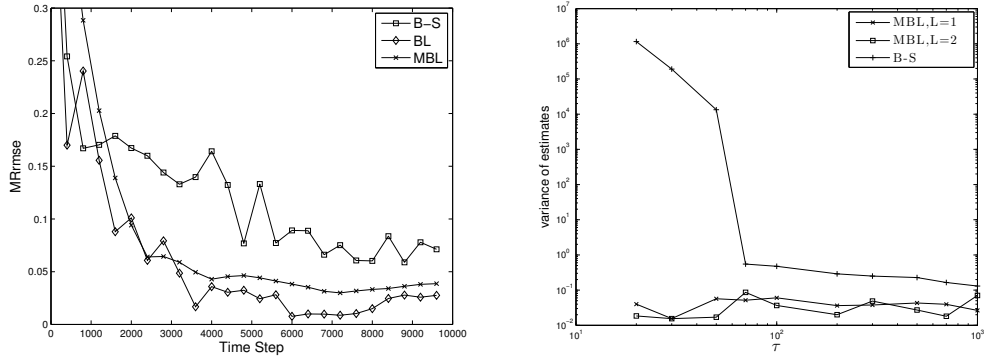


Figure 1: (Linear 2D model with full observation). **Left:** the mean relative root-mean-square error (MRrmse) of the estimates from Berry-Sauer's method (B-S) with $\tau = 2000$, Belanger's method with $L = 1$, and modified Belanger's method with $L = 1, \tau = 1000$. **Right:** Variance of estimates for different τ : Variance of estimates of modified Belanger's method (MBL) with lags $L = 1, 2$ compared to the variance of estimates of Berry-Sauer's method over the last 5000 time steps.

right panel of Figure 1, we show the variances of the estimates of Q and R (based on averaging over the last 5000 time step estimates) as functions of τ . From this numerical test, it is clear that the modified Belanger's method is not only more robust to the choice of τ , it also produces estimates with smaller variances, either using innovations up to lag $L = 1$ or $L = 2$.

Figure 2 shows the comparison results of the original Belanger's method and the modified Belanger's method in the context of partial observations. Here, we show results with $L = 4$ for both methods and $\tau = 1000$ for modified Belanger's method. Note that the results for both methods are comparable in this experiment. In this case, Berry-Sauer's estimation method does not work (results are not shown) since the regression problem in (16) is under determined. Furthermore, this regression problem can become ill-posed for some choice of Γ ; e.g., when $\Gamma = \mathcal{I}$, the regression coefficient for α_2 in (16), that is, $H_{j+1}F_j\Gamma Q_2\Gamma^\top H_j^\top$ is zero and therefore the second diagonal component of Q is unobservable. Indeed, we tested both Belanger's scheme with various lags and found that the estimates are only accurate for $L > 1$. Figure 3 shows the root-mean-square error (RMSE) and the mean of maximum absolute bias (MMAB) of these two versions of Belanger's method. More precisely, we perform 200 independent simulations, each of these assimilates 50,000 steps. These two measuring skills are computed by averaging over these 200 simulations, accounting estimates from the last 5000

steps of 50,000 assimilation steps:

$$\text{RMSE} = \sqrt{\frac{1}{200} \sum_{i=1}^{200} \frac{1}{5000} \sum_{k=45001}^{50000} \|Q_k - Q\|^2 + \|R_k - R\|^2}$$

$$\text{MMAB} = \frac{1}{200} \sum_{i=1}^{200} \max \left\{ \left| \left(\frac{1}{5000} \sum_{k=45001}^{50000} Q_k \right) - Q \right|, \left| \left(\frac{1}{5000} \sum_{k=45001}^{50000} R_k \right) - R \right| \right\},$$

where the maximum is over the entries of these matrices. Notice that the estimates of both methods are accurate according to these measures and the modified Belanger's scheme produces slightly more improved estimates as L increases.

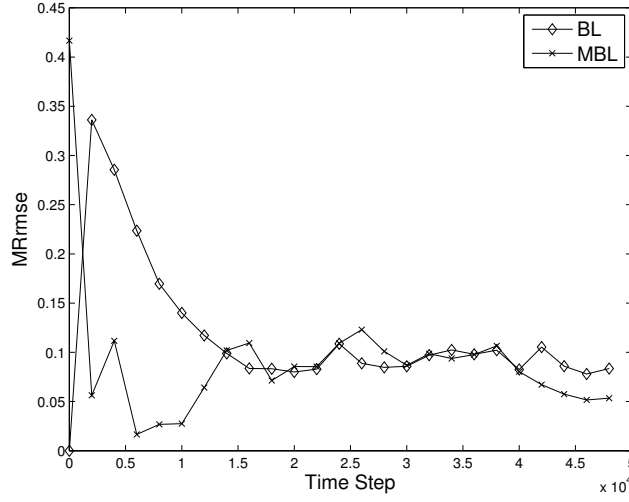


Figure 2: (Linear 2D model with partial observation): The mean relative root-mean-square error of the estimates from Belanger's method with $L = 4$ and modified Belanger's method with $L = 4, \tau = 1000$.

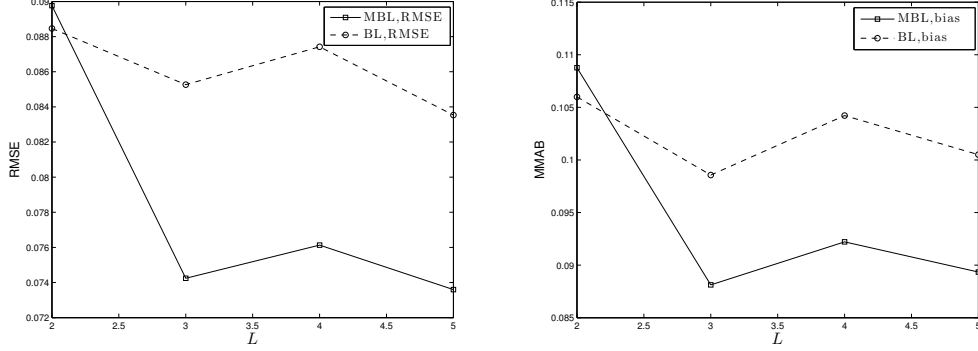


Figure 3: (Linear 2D model with partial observation): Modified Belanger's method (MBL) with $\tau = 1000$ and the original Belanger's method (BL) under linear 2D model with partial observations. Root-mean-square error (left) and mean of maximum absolute bias (right) of QR estimates as functions of L .

3.2. A low-dimensional nonlinear example

In this section, we consider filtering problem of a low-dimensional system of SDE's,

$$\frac{dx}{dt} = Mx + B(x, x) - Dx + \Gamma \dot{W}_t, \quad (22)$$

where $x = (u, v_1, v_2)^\top$, $B(x, x) = (0, auv_2, -auv_1)^\top$, $D = \text{diag}(0, d_1, d_2)$,
 $M = \begin{pmatrix} 0 & \omega & 0 \\ -2\omega & 0 & -\theta \\ 0 & \theta & 0 \end{pmatrix}$, $\Gamma = \begin{pmatrix} 0 & 0 \\ \sigma_1 & 0 \\ 0 & \sigma_2 \end{pmatrix}$ and W_t is the Wiener process with $\mathbb{E}(W_t W_t^\top) = Qt$ where $Q = I_2$. The system in (22), which was called the zeroth level memory model in [15], was derived to model the interaction of a zonal jet u with topographic waves, v_j . In particular, the terms Mx and $B(x, x)$ in (22) are special solutions of the topographic stress model on a two-dimensional periodic domain, truncated up to a total horizontal wavenumber-

one [19, 20], while the linear damping and noises, $-Dx + \Gamma\dot{W}_t$, terms are added to represent the interactions with the unresolved higher-order Rossby modes. The triad model in (22) has some interesting properties, namely, it is geometrically ergodic provided that $d_1, d_2 > 0$, the system has a Gaussian invariant measure, and the systems equilibrium statistics are equivalent to those when ω is replaced by $-\omega$ (see [15] for details).

In the numerical tests below we set $a = 1$, $\omega = \frac{3}{4}$, $\theta = 1$, $d_1 = d_2 = \sigma_1^2 = \sigma_2^2 = \frac{1}{2}$ as in [15]. We choose integration time step and observation time step to be $\delta t = \Delta t = 0.1$. An explicit Euler's scheme is implemented to integrate (22). Here, we implement the parameter estimation method with ETKF (see Algorithm 2 for details) with an ensemble of size $N_e = 16$. In the context of full observations, $H_j = \mathcal{I}_3$ is the identity matrix, and $R = 0.257\mathcal{I}_3\Delta t$ is a diagonal matrix (the observation noise amplitude roughly corresponds to 10% of the variance of u). On the other hand, in the context of partial observations $H_j = (1, 0, 0)$ and $R = 0.257\Delta t$ is a scalar. Since Q and R are diagonal in both situations, we naturally parameterize them by their diagonal components, exactly as in (20).

In Figure 4 (left panel), we compare the performance in the context of full observations. Notice that the relative errors of all three methods are comparable. For this experiment, we set $\tau = 100$ for the modified Belanger's method and $\tau = 1000$ for Berry-Sauer's method so the estimates have small variances. For a fair comparison, we also set $L = 1$ for both the original and modified Belanger's methods. While the relative errors in both versions of Belanger's methods decay faster than that of Berry-Sauer's method, notice that the relative error of the original Belanger's method decays faster than

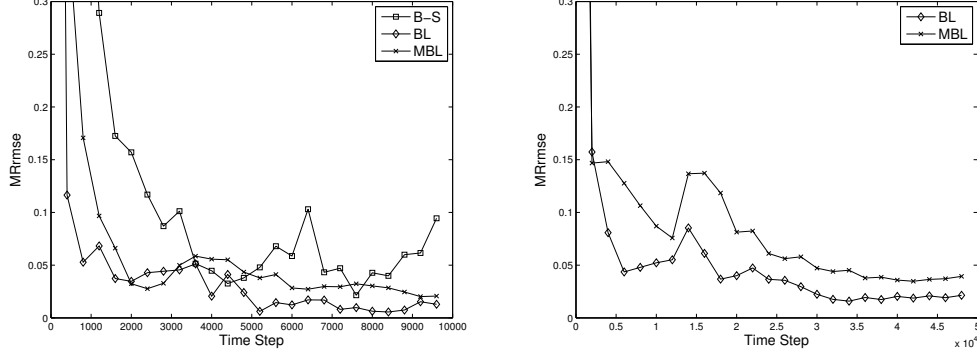


Figure 4: **Left:** (triad model with full observation) the mean relative root-mean-square error of the estimates from Berry-Sauer's method with $\tau = 1000$, Belanger's method with $L = 1$, and Modified Belanger's method with $L = 1, \tau = 100$. **Right:** (triad model with partial observations) the mean relative root-mean-square error of estimates from Belanger's method with $L = 8$ and Modified Belanger's method with $L = 8, \tau = 1000$.

that of the modified Belanger's method. We speculate that this is because the cost function in (13) is defined with a more appropriate norm, as mentioned in Section 2.1.2.

In the context of partial observations, only the first component of the state variables is observed. Again we can not solve Berry-Sauer's least square problem in (16) since it is underdetermined. The right panel of Figure 4 shows the estimates from the two versions of Belanger's method with lag $L = 8$ and $\tau = 1000$. Notice that the relative errors of both methods decay slower when only partial observations are available.

3.3. A stochastically forced 40-dimensional Lorenz-96 example

In this section, we compare the proposed modified Belanger’s method only to Berry-Sauer’s method on a relatively higher-dimensional problems, the 40-dimensional Lorenz-96 model [21], which has been routinely used to validate data assimilation schemes. We ignore showing numerical results with the original Belanger’s method since the computational cost significantly increases as the number of observations, m , becomes large. In our experiment, we follow [14], forcing the Lorenz-96 model [21] with Gaussian white noises. In particular, the system of the stochastically forced Lorenz-96 model is given by:

$$\frac{dx_i}{dt} = -x_{i-2}x_{i-1} + x_{i-1}x_{i+1} - x_i + F + \Gamma_i \dot{W}_t, \quad (23)$$

where Γ_i denotes the i th row of the matrix Γ , which we will set as an identity matrix in our numerical experiments below, and the Wiener process W_t has covariance $\mathbb{E}(W_t W_t^\top) = \hat{Q}t$. We use the standard setting for this model with $F = 8$ and integration step size, $\delta t = 0.05$. The deterministic part of (23) is integrated with a fourth-order Runge-Kutta method while the stochastic part is integrated with the standard Euler’s scheme. In our numerical experiments, we consider sparse, 20 equally spaced, observations of the state variables for every N integration time steps, i.e. $\Delta t = N\delta t$. We generate the true covariance matrix \hat{Q} randomly in the way that the eigenvalue of \hat{Q} distribute uniformly between 0.1 and 1. The observation error covariance R is generated in the same way, but multiplied by a scalar so that we can control the ratio of the error covariances, $\text{tr}(R)/\text{tr}(Q)$, where $Q = \hat{Q}\delta t$ is what we will estimate. In particular, when $\text{tr}(Q) = \text{tr}(R)$ the magnitude of

R is about 0.025 which is about of the same magnitude as that used in [22]. For this nonlinear example, we will apply the modified Belanger's scheme with the ETKF algorithm (2) with an ensemble of size $N_e = 50$ and a total number of 50000 assimilation steps. We parameterize Q and R as in (20), dividing matrices the matrix Q into 4×4 blocks:

$$Q = \begin{pmatrix} \mathcal{B}_{1,1} & \mathcal{B}_{1,2} & \dots & \mathcal{B}_{1,10} \\ \mathcal{B}_{2,1} & \mathcal{B}_{2,2} & \dots & \mathcal{B}_{2,10} \\ \vdots & & & \\ \mathcal{B}_{10,1} & \mathcal{B}_{10,2} & \dots & \mathcal{B}_{10,10} \end{pmatrix}, \text{ and let } Q_s = \begin{pmatrix} 0 & \dots & \dots & \dots & \dots & 0 \\ \vdots & & & & & \\ 0 & \dots & \dots & \mathcal{B}_{s_i, s_j} & \dots & 0 \\ \vdots & & & & & \\ 0 & \dots & \mathcal{B}_{s_j, s_i} & \dots & 0 & 0 \\ \vdots & & & & & \\ 0 & \dots & \dots & \dots & \dots & 0 \end{pmatrix},$$

where s_i and s_j are proper subindexes corresponding to s . Hence there are $N_Q = 55$ parameters for Q . On the other hand, we do not parameterize R , resulting to $N_R = 210$ parameters for R by symmetry. When we estimate α_s and β_s , $\tau = 10000$ is used for Berry-Sauer's method and $\tau = 1000$ and $L = 1$ or $L = 3$ are used for the modified Belanger's method.

Figure 5 shows that reasonably accurate estimates of the first two components x_1 (one of the observed components) and x_2 (one of the unobserved components) of the state variable can be obtained by ensemble transform Kalman filter incorporated with modified Belanger's method with $N = 1$, $L = 3$, and $\text{tr}(R)/\text{tr}(Q) = 1$. We also include the RMSE of the analysis state.

Next, we will discuss the filter performance for different observation step size, N , and covariance ratio, $\text{tr}(R)/\text{tr}(Q)$. Figures 6-8 show the distribution

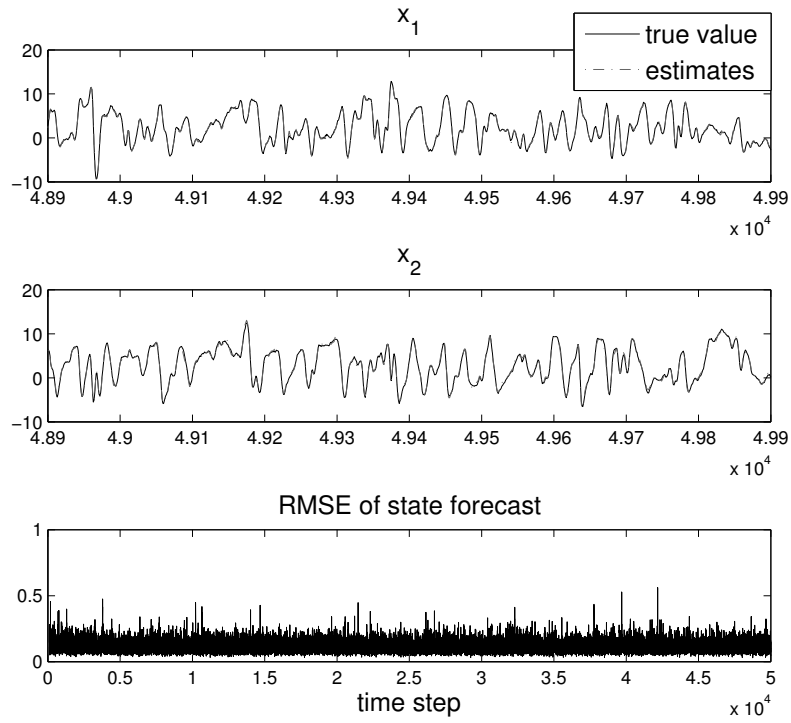


Figure 5: Modified Belanger's scheme: Estimates of x_1 (observed variable) and x_2 (unobserved variable) from the 48900th time step to the 49900th time step, and RMSE of the analysis state.

of relative errors in Q and R based on estimates from the two methods with different L (for modified Belanger’s method only), respectively. Specifically, the relative error is defined by the average over the last 25000 time steps of the following error in percentage:

$$\text{error in percentage} = \frac{\|\text{estimates} - \text{truth}\|}{\|\text{truth}\|} \times 100, \quad (24)$$

where the “estimates” and “truth” refer to the estimation of Q (or R , respectively) at a specific time step and the true Q (or R , respectively) matrix and $\|\cdot\|$ is the Frobenius norm. Figure 6 shows the relative errors from the modified Belanger’s method with $L = 1$. We notice that the estimations of Q and R have different sensitive regions. More generally, for fixed observation time step $\Delta t = N\delta t$, the estimation of Q is less accurate when the magnitude of R is larger, and vice versa. This result can be understood as follows. Recall that the observational matrices $\mathcal{H}^{(Q)}$ (or $\mathcal{H}^{(R)}$) in (6) (or cf. (43), (44)) for the parameter space are linear functions of the basis of Q (or R). Since we parameterize Q (or R) block-wise by the true value of the sub-blocks of Q (or R), larger magnitude of Q (or R) causes $\mathcal{H}^{(Q)}$ (or $\mathcal{H}^{(R)}$) to have larger entries. Since we solve equation (9) directly by a least-square method, we naturally expect more accurate estimates for the parameters with larger coefficients.

We should note that it is possible to use a more appropriate matrix norm in (9) that is similar to the one proposed in the original Belanger’s method, so that we can avoid the estimation of Q and R to have different precision when their magnitudes are significantly different. However this may also raise the computational cost to the same order of that of the original Belanger’s method, which is what we are trying to avoid. According to the analysis above, it is reasonable to deduce that good estimates of Q can be achieved

by the modified Belanger’s method when the magnitude of R is small relative to Q , and vice versa.

On the other hand, we also found that the estimates of the diagonal elements of Q and R are more accurate in most scenarios. We should note that we have also tested on much larger observation noise error with diagonal component 1 and our method still converges (results are not reported). In fact, this method can be applied to much broader choices of N and $\text{tr}(R)/\text{tr}(Q)$ if the true Q and R are diagonal, which motivates one to find better choices of Q_s and R_s to reduce the sensitivity of the estimates when Q and R have different magnitudes. Furthermore, better choices of Q_s and R_s can reduce the number of unknown parameters, α_s, β_s , which is particularly important for large dimensional problems. In our numerical experiments, none of the methods can work when the number of parameters are larger than the number of product of innovation processes that are being used for the covariance estimation.

In Figure 7, we show the corresponding relative errors of Berry-Sauer’s method. We see that the estimation of Q and R by the method of Berry-Sauer’s is less stable when $\text{tr}(R)/\text{tr}(Q)$ is small. However the estimation of Q of their method is more accurate when $\text{tr}(R)/\text{tr}(Q)$ is large. Notice also that the resulting estimates of Q and R do not have the opposite sensitivity when the ratio of $\text{tr}(R)/\text{tr}(Q)$ are different than 1 as encountered in the modified Belanger’s scheme. We suspect that this may be because they estimate R in (15) and Q in (16) separately.

Figure 8 shows the relative errors of the modified Belanger’s method with larger lags, $L = 3$. We see that in many cases the errors indeed can be

reduced by incorporating more lagged information. For example, the relative errors of the estimates of R can be reduced from 74.49% to 32.10% when L is increased from 1 to 3, for $N = 5$ and $\text{tr}(R)/\text{tr}(Q) = 1$. However, we should also mention that increasing lags do not seem to improve the estimates in some regimes with large N (e.g., $N = 6$ and $\text{tr}(R)/\text{tr}(Q) = 0.2$).

In Figure 9 we show the plot of the root-mean-square errors of Q and R as functions of L , for the regime $N = 5$ and $\text{tr}(R)/\text{tr}(Q) = 1$, a case for which the method of Berry-Sauer's does not work well as can be seen in Figure 7. Again, we find that the error of estimates can be reduced by increasing L . But the improvement is small starting from $L = 3$. We suspect that this is because the entries, that corresponds to lags greater than or equal to 3, in the coefficient matrix $\mathcal{H}^{(Q)}$ and $\mathcal{H}^{(R)}$ are small, as we numerically verified. Hence adding more lags beyond $L = 3$ does not increase too much solvability of equation (9).

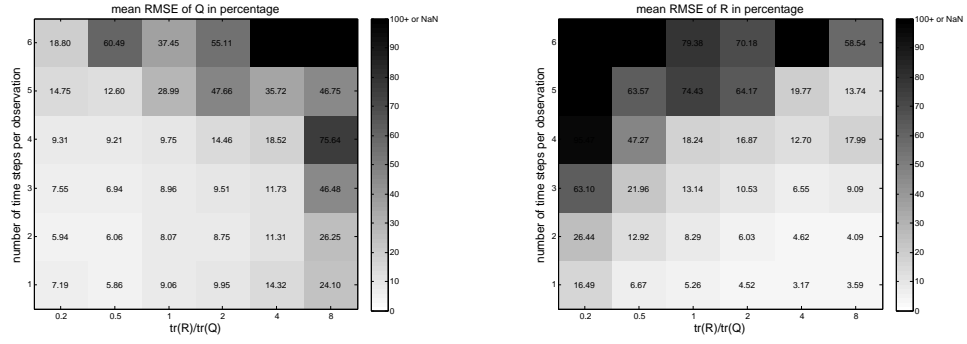


Figure 6: Modified Belanger's method with $L = 1, \tau = 1000$ and Lorenz-96 model: the average of the root-mean-square error (in percentage) of the estimates of Q (left) and R (right) over the last 25000 time steps.

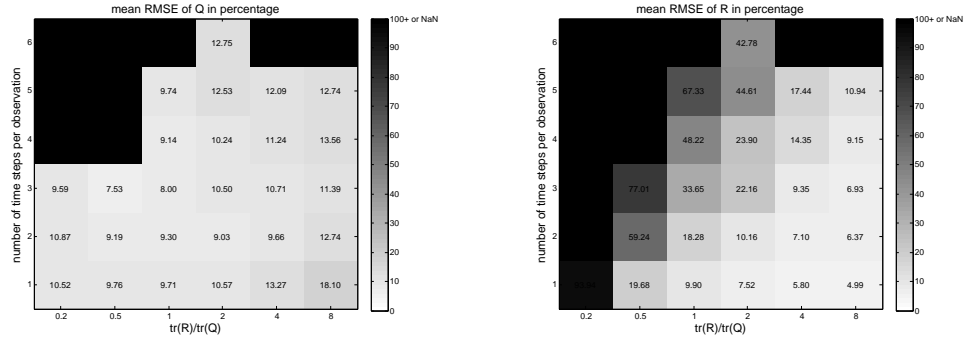


Figure 7: Berry-Sauer's method with $\tau = 10000$ and Lorenz-96 model: the average of the root-mean-square error (in percentage) of the estimates of Q (left) and R (right) over the last 25000 time steps.

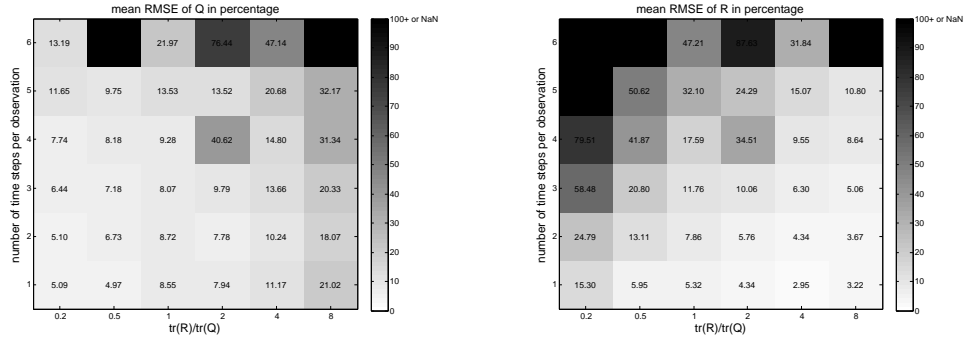


Figure 8: Modified Belanger's method with $L = 3, \tau = 1000$ and Lorenz-96 model: the average of the root-mean-square error (in percentage) of the estimates of Q and R over the last 25000 time steps.

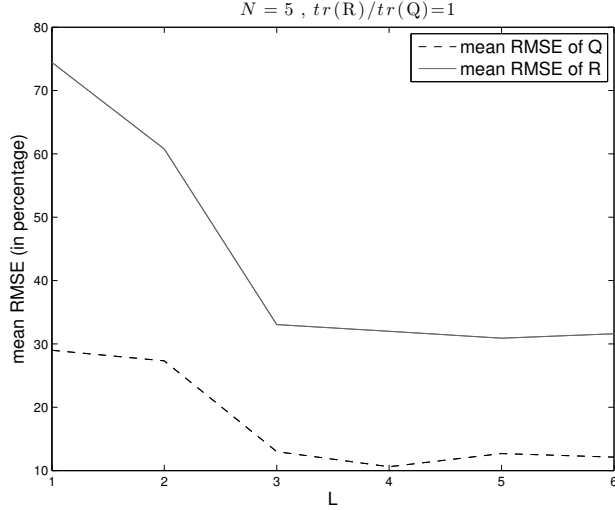


Figure 9: Modified Belanger's method with $L = 1, 2, 3, 4, 5, 6$ and Lorenz-96 model: the average of the root-mean-square error (in percentage) of the estimates of Q and R over the last 25000 time steps.

3.4. Applications on L-96 model using LETKF

In this section we show the numerical results of incorporating the modified Belanger's method in the local ensemble transform Kalman filter (LETKF) ([23, 2]). A brief description of how to apply the modified Belanger's method in the context of LETKF was described in Section 2.2. For comparison purpose, we also show results of implementing the original Belanger's method with LETKF in a similar way. Here we do not show the results with Berry-Sauer's method since they already did it in their paper [14]. We should also note that the incorporation of these methods on other types of localization schemes ([24, 25, 26, 27, 28, 29], etc.) can be nontrivial and beyond the scope of this paper.

In this example, we assume the true model is the original deterministic L96 model in (23) without stochastic noise, $\Gamma_i = 0$. Our goal is to test the potential of the proposed method as an adaptive additive covariance inflation method to mitigate errors due to localization and small ensemble size in addition to estimating R on-the-fly. In particular, one can think of the additive inflation Q as the covariance of a Wiener noise stochastic forcing in the forecast model:

$$\frac{dx_i}{dt} = -x_{i-2}x_{i-1} + x_{i-1}x_{i+1} - x_i + F + \dot{W}_t,$$

where we parameterize:

$$Cov(W_{t+\Delta t}|W_t) =: Q = \begin{pmatrix} q_1 & q_2 & 0 & \dots & 0 & q_2 \\ q_2 & q_1 & q_2 & \dots & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & q_1 & q_2 \\ q_2 & 0 & 0 & \dots & q_2 & q_1 \end{pmatrix}. \quad (25)$$

In this experiment we assume that observations are taken at every site for every $\Delta t = 0.05$, with observational error $R = \mathcal{I}$. To estimate R , we parameterize $R = r\mathcal{I}$, such that the truth is $r = 1$. In total, we have three parameters for Q and R ; $\{q_1, q_2, r\}$. In the following numerical experiments, we set the LETKF with localization radius of 5, i.e., there are 11 sites in each local region. We run the test for 2000 time steps for two ensemble sizes N_e : larger than the local state space with $N_e = 20$ and smaller than the local state space with $N_e = 6$.

The temporal mean RMSE of analysis (MRMSE) and the final estimates of the parameters for Q and R from both the original Belanger's method

	MRMSE	q_1	q_2	r		MRMSE	q_1	q_2	r
BL	0.28	0.01	0.01	1.01	BL	0.77	0.51	0.04	0.9
MBL	0.23	0.01	0.01	1.01	MBL	0.81	0.71	-0.06	0.59

Table 1: Covariance estimates with LETKF with ensemble sizes $N_e = 20$ (left) and $N_e = 6$ (right).

(BL) and the modified Belanger’s method (MBL) are shown in Table 1. It can be seen that the results from both methods are comparable. Compare to the experiments with smaller ensemble size $N_e = 6$, the tests with larger ensemble size $N_e = 20$ produce more accurate state estimates (with smaller MRMSE) and also more accurate estimates of R . Here the estimates for Q are small since the true model is deterministic and the ensemble size is large enough to resolve every possible direction of local error.

In the case of $N_e = 6$, the filter is confronted with a huge sampling error issue, because the ensemble size is much smaller than the dimension of the state variable of each local region. From the numerical results we observe that both methods effectively provide a multiplicative covariance inflation by underestimating R and an additive covariance inflation with nontrivially larger Q . While the MRMSE of the state variables are relatively comparable and still less than the observation error, 1, the weights of these inflations from the two methods are different; the original Belanger scheme provides less overall inflations compared to the modified Belanger’s scheme. We suspect that these differences are due to different norms and cost functions that are minimized in the secondary filters.

4. Summary

We presented a modified version of Belanger’s method to adaptively estimate the system noise covariance Q and observation noise covariance R , which avoids expensive computational cost of the original Belanger’s scheme. We embedded this method into the ensemble transform Kalman filter algorithm as in [15] for filtering nonlinear problems. Similarities and differences between the modified Belanger’s method and those in [10, 14, 16] are discussed. Computationally, the modified Belanger’s scheme applies a cheaper secondary filter; it produces estimates of Q and R based on running averages of linear regression solutions of a new cost function, replacing the secondary recursive Kalman filtering. Although the running average step is similar to the one proposed in [14]), our method is more flexible since its cost function can include product of innovation processes of more than one-lag.

From our numerical results we conclude as follows: While the original Belanger’s scheme produces accurate estimates with faster convergence rate, it is computationally impractical for high-dimensional problems. On low-dimensional problems, we demonstrate that the accuracy of the estimates based on the proposed modified Belanger’s method may be competitive (or even slightly better than) with those of the original Belanger’s method. On the other hand, Berry-Sauer’s method produces the least accurate estimates compared to the two methods even with full observations. For sparse observations, Berry-Sauer’s method sometimes does not work simply because it only uses product of up to one-lag innovation processes. While both the modified Belanger’s and Berry-Sauer’s schemes requires one to prescribe a relaxation coefficient τ , we found that the modified Belanger’s scheme is

not only more robust to variations of this nuisance parameter, but it also produces estimates with smaller variability.

In our numerical test with the Lorenz-96 model we showed that the modified Belanger’s method has wider regimes of accurate estimation compared to Berry-Sauer’s method. In particular, the modified Belanger’s method is more accurate when observation noise amplitude is small relative to system noise amplitude and when observation time step is not too large. Berry-Sauer’s method, on the other hand, has smaller regimes of accurate estimation but it is particularly very accurate when observations noise amplitude is large relative to system noise amplitude. Finally, we also compared the modified and original Belanger’s methods using the local filter with LETKF [2] and tested the potential of using these estimation schemes as an adaptive covariance inflation method in addition to an algorithm for estimating R . We found that their performances are comparable. Both methods significantly reduce the errors even when we use small ensemble size smaller than the dimension of the local state. This encouraging result shows the potential for high-dimensional applications.

Persisting issues for practical implementation of both methods are appropriate choices of Q_s and R_s to reduce the numerical sensitivities and the number of parameters to be estimate. We also numerically found that adding more lags help improving the estimates of the new method in most regimes, however, there seems to be a limit in the improvement of the accuracy of the estimates beyond certain lags. A mathematically more careful analysis to improve our understanding of the approximation property of the modified Belanger’s method is challenging and we leave this out for future studies.

Finally, we should mention that while the scheme was tested in the context of no model error, it will be interesting to see how this scheme will perform in the presence of model error. Obviously, when model error is present, an additional difficulty is to remove biases (or mean model error) from the estimates [30] and recent study suggested that accurate estimation can be obtained when one simultaneously estimates both the mean and covariance error statistics [31], assuming that one knows how to prescribe an appropriate stochastic model as a model error estimator. We plan to test this method to address this issue in our future study.

Acknowledgment

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Appendix A: Detailed formulation

In this appendix we review the mathematical formulation for the original Belanger’s scheme. In particular, consider the following linear filtering problem:

$$x_{j,k} = F_{j,k-1}x_{j,k-1} + \Gamma w_{j,k-1} \quad (26)$$

$$y_{j,1}^o = H_{j,1}x_{j,1} + \xi_{j,1} \quad (27)$$

where we use the same notations as in Section 2. The only difference is that we use two indices j, k , to denote the time point $t_{jN+k} = (jN+k)\delta t$ for

$j \geq 0$ and $1 \leq k \leq N$, indicating that observations are taken for every $N \geq 1$ integration time steps. Our goal is to estimate the state variable $x_{j,1}$, the covariance Q of the system noise w and the covariance R of the observation noise ξ , on the fly.

Since our goal is to compute the coefficient matrix in (6), which is a reasonable approximation for (5) when the Kalman gain matrix K is independent of the noises in the previous time steps, let us assume that this condition holds throughout our derivation below. Recall that given observations $y_{j,1}^o$ and prior mean and covariance estimates, $x_{j,1}^f$ and $B_{j,1}^f$ of the state variable $x_{j,1}$ at time t_{jN+1} , **Kalman filter** computes the posterior estimate $x_{j,1}^a$ and the posterior covariance matrix $B_{j,1}^a$ of $x_{j,1}$, the prior estimate $x_{j,k}^f$ and the prior covariance $B_{j,k}^f$ of $x_{j,k}$ for $2 \leq k \leq N+1$ in the following way:

$$\left\{ \begin{array}{l} K_{j,1} = B_{j,1}^f H_{j,1}^\top (\tilde{R} + H_{j,1} B_{j,1}^f H_{j,1}^\top)^{-1} \\ x_{j,1}^a = x_{j,1}^f + K_{j,1} (y_{j,1}^o - H_{j,1} x_{j,1}^f) \\ B_{j,1}^a = (\mathcal{I} - K_{j,1} H_{j,1}) B_{j,1}^f \\ x_{j,2}^f = F_{j,1} x_{j,1}^a \\ B_{j,2}^f = F_{j,1} B_{j,1}^a F_{j,1}^\top + \Gamma \tilde{Q} \Gamma^\top \\ x_{j,k+1}^f = F_{j,k} x_{j,k}^f \quad \text{for } k = 2, \dots, N \\ B_{j,k+1}^f = F_{j,k} B_{j,k}^a F_{j,k}^\top + \Gamma \tilde{Q} \Gamma^\top \quad \text{for } k = 2, \dots, N \end{array} \right. \quad (28)$$

where \tilde{Q} and \tilde{R} depends on our knowledge of the true system. If \tilde{Q} and \tilde{R} are different from the true value of Q and R the estimates of $x_{j,k}$ would be suboptimal. Define the innovation sequence

$$v_{j,1} := y_{j,1}^o - H_{j,1} x_{j,1}^f. \quad (29)$$

Based on equations (28), we have:

$$\begin{aligned}
\Delta x_{j,1}^f &:= x_{j,1} - x_{j,1}^f \\
&= F_{j-1,N} x_{j-1,N} + \Gamma w_{j-1,N} - F_{j-1,N} x_{j-1,N}^f \\
&= F_{j-1,N} F_{j-1,N-1} (x_{j-1,N-1} - x_{j-1,N-1}^f) + \Gamma w_{j-1,N} + F_{j-1,N} \Gamma w_{j-1,N-1} \\
&= \dots \\
&= \mathbf{F}_{j-1,1}^{j,1} (x_{j-1,1} - x_{j-1,1}^a) \\
&\quad + \mathbf{F}_{j,1}^{j,1} \Gamma w_{j-1,N} + \mathbf{F}_{j-1,N}^{j,1} \Gamma w_{j-1,N-1} + \dots + \mathbf{F}_{j-1,2}^{j,1} \Gamma w_{j-1,1},
\end{aligned} \tag{30}$$

where $\mathbf{F}_{j_2,k_2}^{j_1,k_1}$ denotes the forward operator from time point $t_{j_1N+k_1}$ to time point $t_{j_2N+k_2}$:

$$\mathbf{F}_{j_1,k_1}^{j_2,k_2} = \begin{cases} \mathcal{I} & \text{if } j_1N + k_1 = j_2N + k_2, \\ \prod_{i=j_1N+k_1}^{j_2N+k_2} F_{i_j,i_k} & \text{if } j_2N + k_2 > j_1N + k_1. \end{cases} \tag{31}$$

where i_j, i_k are proper subindexes corresponding to time point t_i . We can now write (30) in a compact form,

$$\Delta x_{j,1}^f = \mathcal{U}_{j-1} \Delta x_{j-1,1}^f - \mathcal{G}_{j-1}^\xi + \mathcal{F}_{j-1}^w, \tag{32}$$

where

$$\begin{cases} \mathcal{U}_{j-1} := \mathbf{F}_{j-1,1}^{j,1} (I - K_{j-1,1} H_{j-1,1}) \\ \mathcal{G}_{j-1}^\xi := \mathbf{F}_{j-1,1}^{j,1} K_{j-1,1} \xi_{j-1,1} \\ \mathcal{F}_{j-1}^w := \mathbf{F}_{j,1}^{j,1} \Gamma w_{j-1,N} + \mathbf{F}_{j-1,N}^{j,1} \Gamma w_{j-1,N-1} + \dots + \mathbf{F}_{j-1,2}^{j,1} \Gamma w_{j-1,1} \end{cases} \tag{33}$$

Let's rewrite (32) in a recursive form,

$$\begin{aligned}
\Delta x_{j,1}^f &= \mathcal{U}_{j-1}\mathcal{U}_{j-2}\Delta x_{j-2,1}^f - (\mathcal{G}_{j-1}^\xi + \mathcal{U}_{j-1}\mathcal{G}_{j-2}^\xi) + (\mathcal{F}_{j-1}^w + \mathcal{U}_{j-1}\mathcal{F}_{j-2}^w) \\
&= \dots \\
&= \left(\prod_{i=1}^j \mathcal{U}_{j-i}\right)\Delta x_{0,1}^f - \mathcal{G}_{(j)}^\xi + \mathcal{F}_{(j)}^w,
\end{aligned} \tag{34}$$

where

$$\mathcal{G}_{(j)}^\xi = \mathcal{G}_{j-1}^\xi + \mathcal{U}_{j-1}\mathcal{G}_{j-2}^\xi + \dots + \mathcal{U}_{j-1}\dots\mathcal{U}_1\mathcal{G}_0^\xi, \tag{35}$$

$$\mathcal{F}_{(j)}^w = \mathcal{F}_{j-1}^w + \mathcal{U}_{j-1}\mathcal{F}_{j-2}^w + \dots + \mathcal{U}_{j-1}\dots\mathcal{U}_1\mathcal{F}_0^w. \tag{36}$$

Since $\xi_{j,k}$ and $w_{j,k}$ are i.i.d. standard normal variables and they are also independent of $\Delta x_{0,1}^f$, and since we assume, in this appendix, that Kalman gain matrices $K_{j,k}$ are independent to these noises, $\xi_{j,k}$ and $w_{j,k}$ at time less than t_{jN+1} , we would have:

$$\begin{aligned}
\mathbb{E}[\Delta x_{j,1}^f(\Delta x_{j-l,1}^f)^\top] &= \left(\prod_{i=1}^j \mathcal{U}_{j-i}\right)\mathbb{E}[\Delta x_{0,1}^f(\Delta x_{0,1}^f)^\top] \left(\prod_{i=1}^{j-l} \mathcal{U}_{j-l-i}\right)^\top \\
&\quad + \mathbb{E}[\mathcal{F}_{(j)}^w(\mathcal{F}_{(j-l)}^w)^\top] + \mathbb{E}[\mathcal{G}_{(j)}^\xi(\mathcal{G}_{(j-l)}^\xi)^\top]
\end{aligned} \tag{37}$$

where the expectation is taken with respect to each realization of w and ξ .

Given that the system is asymptotically stable, $\prod_{i=1}^{j-l} \mathcal{U}_{j-i}$ decays exponentially fast [10]. Hence the first term in (37) is small when $j-l$ is large enough.

Further it is not hard to see that the last two terms in (37) are linear functions

of Q or R respectively, meaning that if we linearly parameterize $Q = \sum_{s=1}^{N_Q} \alpha_s Q_s$

and $R = \sum_{s=1}^{N_R} \beta_s R_s$ using some prescribed basis Q_s, R_s , we can write the last

two terms of (37) as a linear function of α_s and β_s :

$$\mathbb{E}[\mathcal{F}_{(j)}^w (\mathcal{F}_{(j-l)}^w)^\top] = \sum_{s=1}^{N_Q} \alpha_s \Phi_{j,l,s}^{(Q)} \quad (38)$$

$$\mathbb{E}[\mathcal{G}_{(j)}^\xi (\mathcal{G}_{(j-l)}^\xi)^\top] = \sum_{s=1}^{N_R} \beta_s \Phi_{j,l,s}^{(R)}. \quad (39)$$

Belanger pointed out that the matrix $\Phi_{j,l,s}^{(Q)}$ and $\Phi_{j,l,s}^{(R)}$ can be computed recursively [10]:

$$\Phi_{j,l,s}^{(Q)} = \begin{cases} \mathcal{U}_{j-1} \Phi_{j-1,l-1,s}^{(Q)} & \text{if } l > 0 \\ \mathcal{U}_{j-1} \Phi_{j-1,0,s}^{(Q)} \mathcal{U}_{j-1}^\top + \Gamma Q_s \Gamma^\top & \text{if } l = 0, N = 1 \\ \mathcal{U}_{j-1} \Phi_{j-1,0,s}^{(Q)} \mathcal{U}_{j-1}^\top + \Gamma Q_s \Gamma^\top + \sum_{i=1}^{N-1} \mathbf{F}_{j-1,i+1}^{j,1} \Gamma Q_s \Gamma^\top (\mathbf{F}_{j-1,i+1}^{j,1})^\top & \text{if } l = 0, N > 1 \end{cases} \quad (40)$$

$$\Phi_{j,l,s}^{(R)} = \begin{cases} \mathcal{U}_{j-1} \Phi_{j-1,l-1,s}^{(R)} & \text{if } l > 0 \\ \mathcal{U}_{j-1} \Phi_{j-1,0,s}^{(R)} \mathcal{U}_{j-1}^\top + \mathcal{S}_{j-1} R_s \mathcal{S}_{j-1}^\top & \text{if } l = 0, \end{cases} \quad (41)$$

where we define $\mathcal{S}_{j-1} := \mathbf{F}_{j-1,1}^{j,1} K_{j-1,1}$. Based on equations (29), (37)-(41),

we have

$$\begin{aligned}
\mathbb{E}(v_{j,1}v_{j-l,1}^\top) &= H_{j,1}\mathbb{E}[\Delta x_{j,1}^f(\Delta x_{j-l,1}^f)^\top]H_{j-l,1}^\top + H_{j,1}\mathbb{E}[\Delta x_{j,1}^f\xi_{j-l,1}^\top] \\
&= \sum_{s=1}^{N_Q} \alpha_s H_{j,1}\Phi_{j,l,s}^{(Q)}H_{j-l,1}^\top + \sum_{s=1}^{N_R} \beta_s H_{j,1}\Phi_{j,l,s}^{(R)}H_{j-l,1}^\top \\
&\quad + \begin{cases} \sum_{s=1}^{N_R} \beta_s R_s & \text{if } l = 0 \\ -\sum_{s=1}^{N_R} \beta_s H_{j,1}\mathcal{S}_{j-1}R_s & \text{if } l = 1 \\ -\sum_{s=1}^{N_R} \beta_s H_{j,1}\mathcal{U}_{j-1}\dots\mathcal{U}_{j-l+1}\mathcal{S}_{j-l}R_s & \text{if } l > 1. \end{cases} \quad (42)
\end{aligned}$$

and we can define a linear observation operator for Q and R with coefficients:

$$\mathcal{H}_{j,l,s}^{(Q)} := H_{j,1}\Phi_{j,l,s}^{(Q)}H_{j-l,1}^\top \quad (43)$$

$$\mathcal{H}_{j,l,s}^{(R)} := H_{j,1}\Phi_{j,l,s}^{(R)}H_{j-l,1}^\top + \begin{cases} R_s & \text{if } l = 0 \\ -H_{j,1}\mathcal{S}_{j-1}R_s & \text{if } l = 1 \\ -H_{j,1}\mathcal{U}_{j-1}\dots\mathcal{U}_{j-l+1}\mathcal{S}_{j-l}R_s & \text{if } l > 1, \end{cases} \quad (44)$$

so that (42) can be conveniently written as

$$\mathbb{E}(v_{j,1}v_{j-l,1}^\top) = \sum_{s=1}^{N_Q} \alpha_s \mathcal{H}_{j,l,s}^{(Q)} + \sum_{s=1}^{N_R} \beta_s \mathcal{H}_{j,l,s}^{(R)}, \quad (45)$$

which is exactly (6) in the case when observations are taken every integration time step ($N = 1$).

Appendix B. Pseudo-code

In this appendix, we present a complete pseudo-code of the modified Belanger's method. To make this paper self-contained we also present the ETKF algorithm that we used for filtering stochastic nonlinear systems. This version of ETKF is similar to the one used by [15] and it is a variant of the one formulated earlier by [2]. We should also mention that this pseudo-code is not optimal so one may need to optimize it carefully for high-dimensional problems. The following notations are needed:

- $n \in \mathbb{N}$: the dimension of state variable;
- $m \in \mathbb{N}$: the dimension of observation;
- $N \in \mathbb{N}$: number of time steps per observation;
- $N_e \in \mathbb{N}$: the ensemble size;
- $n_s \in \mathbb{N}$: the dimension of system noise w_k ;
- $x_{j,k} \in \mathbb{R}^{n \times 1}$: the true state variable at the $jN + k$ -th time step;
- $X_{j,k}^{f,i} \in \mathbb{R}^{n \times 1}$: the i -th ensemble member of prior estimate of state variable at the $jN + k$ -th time step, for $i = 1, \dots, N_e$;
- $X_{j,k}^{df,i} \in \mathbb{R}^{n \times 1}$: the i -th ensemble member of deterministic forecast of state variable at the $jN + k$ -th time step, for $i = 1, \dots, N_e$;
- $\bar{X}_{j,k}^f \in \mathbb{R}^{n \times 1}$: ensemble mean of prior estimate of state variable at the $jN + k$ -th time step;
- $X_{j,k}^{a,i} \in \mathbb{R}^{n \times 1}$: the i -th ensemble member of posterior estimate of state variable at the $jN + k$ -th time step, for $i = 1, \dots, N_e$;
- $\bar{X}_{j,k}^a \in \mathbb{R}^{n \times 1}$: ensemble mean of posterior estimate of state variable at the $jN + k$ -th time step;
- $v_{j,1} \in \mathbb{R}^{m \times 1}$: the innovation at the $jN + 1$ 'st time step;
- $B_{j,k}^f \in \mathbb{R}^{n \times n}$: prior covariance of state variable at the $jN + k$ -th time step;
- $B_{j,1}^a \in \mathbb{R}^{n \times n}$: posterior covariance of the state variable at the $jN + 1$ 'st time step;
- $K_{j,k} \in \mathbb{R}^{n \times m}$: the Kalman gain at the $jN + k$ -th time step;
- $h_{j,1}$: observational operator at the $jN + 1$ 'st time step;
- $H_{j,1} \in \mathbb{R}^{m \times n}$: the linear version of $h_{j,1}$;
- $f_{j,k}$: the nonlinear deterministic model operator that transmits state variable from the $jN + k$ -th time step to the $jN + k + 1$ 'st time step;
- $F_{j,k} \in \mathbb{R}^{n \times n}$: the linear version of $f_{j,k}$;
- $Q \in \mathbb{R}^{n_s \times n_s}$: the covariance of system noise w_k ;
- $\Gamma \in \mathbb{R}^{n \times n_s}$: the coefficient of system noise;
- $R \in \mathbb{R}^{m \times m}$: the covariance of observation noise ξ_k .
- $\Phi_{j,l,s}^{(Q)}$ and $\Phi_{j,l,s}^{(R)}$: the matrices defined by (38) and (39) for $l = 0, \dots, L$;
- $\mathcal{H}_{j,l,s}^{(Q)}$ and $\mathcal{H}_{j,l,s}^{(R)}$: the matrices defined by (45) for $l = 0, \dots, L$;
- $\mathcal{H}_{j,l,s}^{(Q)\text{sum}}$ and $\mathcal{H}_{j,l,s}^{(R)\text{sum}}$: the sum of $\mathcal{H}_{j,l,s}^{(Q)}$ and $\mathcal{H}_{j,l,s}^{(R)}$, respectively, from time $t_{(L+1)N+1}$ to t_{jN+1} ;
- $\mathcal{Y}_{j,l}^{(QR)\text{sum}}$: the sum of $v_{j,1} v_{j-l,1}^\top$ from $t_{(L+1)N+1}$ up to time t_{jN+1} ;
- N_Q : number of parameters for Q ;
- N_R : number of parameters for R ;
- \mathcal{Q}_s : the basis of parameterization of Q , for $s = 1, \dots, N_Q$;
- \mathcal{R}_s : the basis of parameterization of R , for $s = 1, \dots, N_R$;
- Q_j : the estimation of Q that is used in the primary filter at the $jN + 1$ 'st time step;
- R_j : the estimation of R that is used in the primary filter at the $jN + 1$ 'st time step;
- τ : the relaxation coefficient in (10) and (11).

Algorithm 1 Covariance Estimation at the $jN + 1$'s Time Step

Input: $v_{j-l,1}, B_{j-l,1}^f, K_{j-l,1}, F_{j-l-1,k}, H_{j-l,1}, \mathcal{Q}_s, \mathcal{R}_s, \Gamma, \alpha_{s,j-1}, Q_{j-1}, R_{j-1}, \beta_{s,j-1},$
 $\mathcal{U}_{j-l-1}, \mathcal{S}_{j-l-1}, \Phi_{j-1,l,s}^{(Q)}, \Phi_{j-1,l,s}^{(R)}, \mathcal{H}_{j-1,l,s}^{(Q)\text{sum}}, \mathcal{H}_{j-1,l,s}^{(R)\text{sum}}, \mathcal{Y}_{j-1,l}^{(QR)\text{sum}}, \tau$, for $1 \leq s \leq$
 N_Q or $N_R, 0 \leq l \leq L$

Output: $\alpha_{s,j}, \beta_{s,j}, Q_j, R_j, \Phi_{j,l,s}^{(Q)}, \Phi_{j,l,s}^{(R)}, \mathcal{Y}_{j,l}^{(QR)\text{sum}}, \mathcal{H}_{j,l,s}^{(Q)\text{sum}}, \mathcal{H}_{j,l,s}^{(R)\text{sum}}$, for $0 \leq l \leq$
 L

```

1: if  $j < L + 1$  then    % do not do anything for the first  $L$  time steps
2:    $\alpha_{s,j} \leftarrow \alpha_{s,j-1}$    for  $s = 1, \dots, N_Q$ 
3:    $\beta_{s,j} \leftarrow \beta_{s,j-1}$    for  $s = 1, \dots, N_R$ 
4:    $Q_j \leftarrow Q_{j-1}$ 
5:    $R_j \leftarrow R_{j-1}$ 
6:    $\Phi_{j,l,s}^{(Q)} \leftarrow \Phi_{j-1,l,s}^{(Q)}$    for  $l = 0, \dots, L$  and  $s = 1, \dots, N_Q$ 
7:    $\Phi_{j,l,s}^{(R)} \leftarrow \Phi_{j-1,l,s}^{(R)}$    for  $l = 0, \dots, L$  and  $s = 1, \dots, N_R$ 
8:    $\mathcal{Y}_{j,l}^{(QR)\text{sum}} \leftarrow \mathcal{Y}_{j-1,l}^{(QR)\text{sum}}$    for  $l = 0, \dots, L$ 
9:    $\mathcal{H}_{j,l,s}^{(Q)\text{sum}} \leftarrow \mathcal{H}_{j-1,l,s}^{(Q)\text{sum}}$    for  $l = 0, \dots, L$  and  $s = 1, \dots, N_Q$ 
10:   $\mathcal{H}_{j,l,s}^{(R)\text{sum}} \leftarrow \mathcal{H}_{j-1,l,s}^{(R)\text{sum}}$    for  $l = 0, \dots, L$  and  $s = 1, \dots, N_R$ 
11: else
12:   for  $l = 0$  to  $L$  do
13:      $\mathcal{Y}_{j,l}^{(QR)\text{sum}} \leftarrow \mathcal{Y}_{j-1,l}^{(QR)\text{sum}} + v_{j,1} v_{j-l,1}^\top$    % Compute  $\sum_{j=L+1}^J v_j v_{j-l}^\top$  in (9)
14:     if  $l = 0$  then
15:       for  $s = 1$  to  $N_Q$  do
16:          $\Phi_{j,l,s}^{(Q)} \leftarrow \mathcal{U}_{j-1} \Phi_{j-1,0,s}^{(Q)} \mathcal{U}_{j-1}^\top + \mathcal{Q}_s$ 
17:          $\mathbf{F}_{j,1}^{j,1} \leftarrow I$ 

```

```

18:      for  $k = N$  to 2 do
19:           $\mathbf{F}_{j-1,k}^{j,1} \leftarrow \mathbf{F}_{j-1,k+1}^{j,1} F_{j-1,k}$ 
20:           $\Phi_{j,1,s}^{(Q)} \leftarrow \Phi_{j-1,1,s}^{(Q)} + \mathbf{F}_{j-1,k}^{j,1} \Gamma \mathcal{Q}_s \Gamma^\top (\mathbf{F}_{j-1,k}^{j,1})^\top$ 
21:      end for
22:       $\mathcal{H}_{\text{temp},s}^{(Q)} \leftarrow H_{j,1} \Phi_{j,1,s}^{(Q)} H_{j,1}^\top$  % Compute  $\mathcal{H}_{j,l,s}^{(Q)}$  in (9)
23:  end for
24:  for  $s = 1$  to  $N_R$  do
25:       $\Phi_{j,1,s}^{(R)} \leftarrow \mathcal{U}_{j-1} \Phi_{j,1,s}^{(R)} \mathcal{U}_{j-1}^\top + \mathcal{S}_{j-1} \mathcal{R}_s \mathcal{S}_{j-1}^\top$ 
26:       $\mathcal{H}_{\text{temp},s}^{(R)} \leftarrow H_{j,1} \Phi_{j,1,s}^{(R)} H_{j,1}^\top + \mathcal{R}_s$ 
27:  end for
28:  else
29:      for  $s = 1$  to  $N_Q$  do
30:           $\Phi_{j,l,s}^{(Q)} \leftarrow \mathcal{U}_{j-1} \Phi_{j-1,l-1,s}^{(Q)}$ 
31:           $\mathcal{H}_{\text{temp},s}^{(Q)} \leftarrow H_{j,1} \Phi_{j,l,s}^{(Q)} H_{j,1}^\top$ 
32:      end for
33:      for  $s = 1$  to  $N_R$  do
34:           $\Phi_{j,1,s}^{(R)} \leftarrow \mathcal{U}_{j-1} \Phi_{j-1,l-1,s}^{(R)}$ 
35:          if  $l = 1$  then % Compute  $\mathcal{H}_{j,l,s}^{(R)}$  in (9)
36:               $\mathcal{H}_{\text{temp},s}^{(R)} \leftarrow H_{j,1} \Phi_{j,l,s}^{(R)} H_{j-l,1}^\top - H_{j,1} \mathcal{S}_{j-1} \mathcal{R}_s$ 
37:          else
38:               $\mathcal{H}_{\text{temp},s}^{(R)} \leftarrow H_{j,1} \Phi_{j,l,s}^{(R)} H_{j-l,s}^\top - H_{j,1} \mathcal{U}_{j-1} \dots \mathcal{U}_{j-l+1} \mathcal{S}_{j-1} \mathcal{R}_s$ 
39:          end if
40:      end for
41:  end if
42:  end for

```

```

43:  % Compute  $\sum_{j=L+1}^J \mathcal{H}_{j,l,s}^{(Q)}$  and  $\sum_{j=L+1}^J \mathcal{H}_{j,l,s}^{(R)}$  in (9)
44:   $\mathcal{H}_{j,l,s}^{(Q)\text{sum}} \leftarrow \mathcal{H}_{j-1,l,s}^{(Q)\text{sum}} + \mathcal{H}_{\text{temp},s}^{(Q)}$ , for  $l = 0, 1, \dots, L$  and  $s = 1, \dots, N_Q$ 
45:   $\mathcal{H}_{j,l,s}^{(R)\text{sum}} \leftarrow \mathcal{H}_{j-1,l,s}^{(R)\text{sum}} + \mathcal{H}_{\text{temp},s}^{(R)}$ , for  $l = 0, 1, \dots, L$  and  $s = 1, \dots, N_R$ 
46:  reshape  $\mathcal{H}_{j,l,s}^{(Q)\text{sum}}$  to get  $\mathbf{h}_{l,s}^{(q)} \in \mathbb{R}^{m^2 \times 1}$  for  $1 \leq s \leq N_Q$  and  $0 \leq l \leq L$ 
47:  reshape  $\mathcal{H}_{j,l,s}^{(R)\text{sum}}$  to get  $\mathbf{h}_{l,s}^{(r)} \in \mathbb{R}^{m^2 \times 1}$  for  $1 \leq s \leq N_R$  and  $0 \leq l \leq L$ 
48:   $\mathfrak{H}_l^{(q)} \leftarrow [\mathbf{h}_{l,1}^{(q)}, \mathbf{h}_{l,2}^{(q)}, \dots, \mathbf{h}_{l,N_Q}^{(q)}]$  for  $l = 0, 1, \dots, L$ 
49:   $\mathfrak{H}_l^{(r)} \leftarrow [\mathbf{h}_{l,1}^{(r)}, \mathbf{h}_{l,2}^{(r)}, \dots, \mathbf{h}_{l,N_R}^{(r)}]$  for  $l = 0, 1, \dots, L$ 
50:   $\mathfrak{H}^{(q)} \leftarrow \begin{pmatrix} \mathbf{h}_0^{(q)} \\ \mathbf{h}_1^{(q)} \\ \vdots \\ \mathbf{h}_L^{(q)} \end{pmatrix}$ ,  $\mathfrak{H}^{(r)} \leftarrow \begin{pmatrix} \mathbf{h}_0^{(r)} \\ \mathbf{h}_1^{(r)} \\ \vdots \\ \mathbf{h}_L^{(r)} \end{pmatrix}$ ,  $\mathfrak{Y}^{(qr)} \leftarrow \begin{pmatrix} \mathcal{Y}_{j,0}^{(QR)\text{sum}} \\ \mathcal{Y}_{j,1}^{(QR)\text{sum}} \\ \vdots \\ \mathcal{Y}_{j,L}^{(QR)\text{sum}} \end{pmatrix}$ 
51:   $\mathfrak{H}^{(qr)} \leftarrow [\mathfrak{H}^{(q)}, \mathfrak{H}^{(r)}]$ 
52:   $\Lambda^{(qr)} \leftarrow ((\mathfrak{H}^{(qr)})^\top \mathfrak{H}^{(qr)})^\dagger (\mathfrak{H}^{(qr)})^\top \mathfrak{Y}^{(qr)}$ , where  $\dagger$  denotes the matrix pseudo-
inverse. % Solve (9) for the covariance parameters using least square
method
53:  % Temporal smoothing of covariance parameters. Refer to (10) and (11)
54:   $\alpha_{s,j} \leftarrow \alpha_{s,j-1} + 1/\tau(\Lambda_s^{(qr)} - \alpha_{s,j-1})$  for  $s = 1, \dots, N_Q$ 
55:   $\beta_{s,j} \leftarrow \beta_{s,j-1} + 1/\tau(\Lambda_{s+N_Q}^{(qr)} - \beta_{s,j-1})$  for  $s = 1, \dots, N_R$ 
56:   $Q_j \leftarrow \sum_{s=1}^{N_Q} \alpha_{s,j} \mathcal{Q}_s$ ,  $R_j \leftarrow \sum_{s=1}^{N_R} \beta_{s,j} \mathcal{R}_s$  % Construct  $Q$  and  $R$  from the
newly estimated parameters
57: end if

```

Algorithm 2 Ensemble Transform Kalman Filter (for stochastic nonlinear systems) from the $(jN + 1)$ 'st Time Step to $(j + 1)N + 1$ 'st Time Step

Input: $y_{j,1}^o, X_{j,1}^{f,i}, B_{j,1}^f, f_{j,k}, h_{j,1}, Q, R, \Gamma$

Output: $X_{j+1,1}^{f,i}, B_{j+1,1}^f, F_{j,k}, H_{j,1}, K_{j,1}, B_{j,1}^a$ for $1 \leq k \leq N$

1: % ETKF is widely known and has many different versions. For a detailed description of this version please refer to [2, 32]

$$2: \bar{X}_{j,1}^f \leftarrow \frac{1}{N_e} \sum_{i=1}^{N_e} X_{j,1}^{f,i}$$

$$3: U_{j,1}^{(i)} \leftarrow X_{j,1}^{f,i} - \bar{X}_{j,1}^f, \quad \text{for } i = 1, 2, \dots, N_e.$$

$$4: Y_{j,1}^{f,i} \leftarrow h_{j,1}(X_{j,1}^{f,i}), \quad \text{for } i = 1, 2, \dots, N_e.$$

$$5: U \leftarrow [U_{j,1}^{f,1}, \dots, U_{j,N_e}^{f,N_e}]$$

$$6: \bar{Y}_{j,1}^f \leftarrow \frac{1}{N_e} \sum_{i=1}^{N_e} Y_{j,1}^{f,i}$$

$$7: V_{j,1}^{f,i} \leftarrow Y_{j,1}^{f,i} - \bar{Y}_{j,1}^f, \quad \text{for } i = 1, 2, \dots, N_e$$

$$8: V \leftarrow [V_{j,1}^{f,1}, \dots, V_{j,1}^{f,N_e}]$$

$$9: \boxed{H_{j,1} \leftarrow VU^\dagger} \text{ where } \dagger \text{ refers to the matrix pseudo-inverse.}$$

$$10: J \leftarrow (N_e - 1)I + V^\top R^{-1}V$$

$$11: x \leftarrow J^{-1}V^\top R^{-1}v_{j,1}$$

$$12: \bar{X}_{j,1}^a \leftarrow \bar{X}_{j,1}^f + Ux$$

$$13: \text{Compute the singular value decomposition (SVD) of } J = E_1 D_1 E_1^\top$$

$$14: D_2 \leftarrow (N_e - 1)D_1^{-1}$$

$$15: T \leftarrow E_1 \sqrt{D_2} E_1^\top$$

$$16: P_y \leftarrow \frac{1}{N_e - 1} V V^\top + R$$

$$17: P_{xy} \leftarrow \frac{1}{N_e - 1} U V^\top$$

$$18: \boxed{K_{j,1} \leftarrow P_{xy} P_y^{-1}}$$

$$19: U^a \leftarrow UT, \text{ denote the } i\text{-th column of } U^a \text{ by } U^{a,i};$$

$$20: \boxed{B_{j,1}^a \leftarrow U^a (U^a)^\top / (N_e - 1)}$$

$$21: X_{j,1}^{a,i} \leftarrow \bar{X}_{j,1}^a + U^{a,i}, \quad \text{for } i = 1, 2, \dots, N_e.$$

22: $X^{\text{temp}} \leftarrow X_{j,1}^a$, denote the i -th column by $X^{\text{temp},i}$

23: **for** $k = 1$ to N **do**

24: $\bar{X}^{\text{temp}} \leftarrow \frac{1}{N_e} \sum_{i=1}^{N_e} X^{\text{temp},i}$

25: $U^{f,i} \leftarrow X^{\text{temp},i} - \bar{X}^{\text{temp}}$ for $i = 1, 2, \dots, N_e$.

26: $U^f \leftarrow [U^{f,1}, \dots, U^{f,N_e}]$

27: $B^{\text{temp}} \leftarrow \frac{1}{N_e-1} U^f (U^f)^\top$

28: $X^{\text{temp},i} \leftarrow f_{j,k}(X^{\text{temp},i})$

29: $\bar{X}^{\text{temp}} \leftarrow \frac{1}{N_e} \sum_{i=1}^{N_e} X^{\text{temp},i}$

30: $U^{df,i} \leftarrow X^{\text{temp},i} - \bar{X}^{\text{temp}}$ for $i = 1, 2, \dots, N_e$

31: $U^{df} \leftarrow [U^{df,1}, \dots, U^{df,N_e}]$

32: $\boxed{F_{j,k} \leftarrow U^{df} (U^f)^\dagger}$

33: $B^{\text{temp}} \leftarrow \frac{1}{N_e-1} U^f (U^f)^\top + \Gamma Q \Gamma^\top$

34: Independently generate N_e standard normal random vectors $\delta^i \in \mathbb{R}^{n \times 1}$,
 for $1 \leq i \leq N_e$

35: $\bar{\delta} \leftarrow \frac{1}{N_e} \sum_{i=1}^{N_e} \delta^i$

36: $\delta^i \leftarrow \delta^i - \bar{\delta}$ for $i = 1, 2, \dots, N_e$.

37: $\delta \leftarrow [\delta^1, \dots, \delta^{N_e}]$

38: Compute the singular value decomposition of $\frac{1}{N_e-1} \delta \delta^\top = E_3 D_3 E_3^\top$

39: $U^{\text{temp}} \leftarrow \sqrt{B^{\text{temp}}} E_3 (D_3)^{-1} E_3^\top \delta$, denote the i -th column by $U^{\text{temp},i}$

40: $X^{\text{temp},i} \leftarrow \bar{X}^{\text{temp}} + U^{\text{temp},i}$ for $i = 1, 2, \dots, N_e$

41: **end for**

42: $\boxed{X_{j+1,1}^{f,i} \leftarrow X^{\text{temp},i} \text{ for } i = 1, \dots, N_e}$

43: $\boxed{B_{j+1,1}^f \leftarrow B^{\text{temp}}}$

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